| REPORT DOCUMENTATION PAGE | Form Approved OMB NO. 0704-0188 |
|---|---|



| 1. AGENCY USE ONLY *(Leave Blank)* | 2. REPORT DATE | 3. REPORT TYPE AND DATES COVERED |
|---|---|---|
| | 5/20/01 | Final Progress Report, 01 Aug 97 - 01 Oct 00 |

4. TITLE AND SUBTITLE
Ensemble Quantum Computing by Liquid-State NMR Spectroscopy

5. FUNDING NUMBERS
DAAG 55-97-1-0342



6. AUTHOR(S)
Timothy F. Havel
David G. Cory

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Biological Chemistry and Molecular Pharmacology, Harvard Medical School, 240 Longwood Ave., Boston MA 02115
Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING / MONITORING AGENCY REPORT NUMBER
AMSRO-ICA 37521-PH-QC
.24

11. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

12a. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

The goals of this project were to use liquid-state nuclear magnetic resonance (NMR) as a testbed for developing general methods of solving computational problems on ensemble quantum computers, to study the fundamental physics and computer science behind such machines, and to learn how to make optimal use of the trade-offs that their unique capabilities permit us to make. During the three years of this project, we have: (1) developed a library of radio-frequency pulse sequences which allow a rich repertoire of unitary "quantum logic gates" to be implemented by NMR; (2) designed general methods, based on magnetic field gradients, for preparing the "pseudopure" states needed for quantum computing by liquid-state NMR; (3) invented procedures, based on gradients combined with molecular diffusion, by which a wide variety of decoherent processes can be implemented using NMR; (4) used these procedures to perform the first demonstrations of quantum error correction as well as decoherence-free subspaces / systems; (5) used the average Hamiltonian techniques developed many years ago by John Waugh at MIT to implement the first simulations of one quantum system by another, as originally proposed by Richard Feynman. Many of the techniques we have developed in the course of this work promise to be highly useful in other approaches to quantum computing, both by our group as well as many others.

| 14. SUBJECT TERMS | 15. NUMBER OF PAGES 17 |
|---|---|
| | 16. PRICE CODE |

| 17. SECURITY CLASSIFICATION OF REPORT | 18. SECURITY CLASSIFICATION OF THIS PAGE | 19. SECURITY CLASSIFICATION OF ABSTRACT | 20. LIMITATION OF ABSTRACT |
|---|---|---|---|
| UNCLASSIFIED | UNCLASSIFIED | UNCLASSIFIED | UL |

# ENSEMBLE QUANTUM COMPUTING BY LIQUID-STATE NMR SPECTROSCOPY

## FINAL REPORT

TIMOTHY F. HAVEL & DAVID G. CORY

MAY 23, 2001

U.S. ARMY RESEARCH OFFICE

DAAG55-97-1-0342

AMSRO-ICA 37521-PH-QC

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

| REPORT DOCUMENTATION PAGE | Form Approved OMB NO. 0704-0188 |
|---|---|



| 1. AGENCY USE ONLY *(Leave Blank)* | 2. REPORT DATE | 3. REPORT TYPE AND DATES COVERED |
|---|---|---|
| | 5/20/01 | Final Progress Report, 8/15/97 - 9/30/00 |

4. TITLE AND SUBTITLE
Ensemble Quantum Computing by Liquid-State NMR Spectroscopy

5. FUNDING NUMBERS
DAAG 55-97-1-0342

6. AUTHOR(S)
Timothy F. Havel
David G. Cory

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Biological Chemistry and Molecular Pharmacology, Harvard Medical School, 240 Longwood Ave., Boston MA 02115
Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING / MONITORING AGENCY REPORT NUMBER
AMSRO-ICA 37521-PH-QC

11. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

12a. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

The goals of this project were to use liquid-state nuclear magnetic resonance (NMR) as a testbed for developing general methods of solving computational problems on ensemble quantum computers, to study the fundamental physics and computer science behind such machines, and to learn how to make optimal use of the trade-offs that their unique capabilities permit us to make. During the three years of this project, we have: (1) developed a library of radio-frequency pulse sequences which allow a rich repertoire of unitary "quantum logic gates" to be implemented by NMR; (2) designed general methods, based on magnetic field gradients, for preparing the "pseudopure" states needed for quantum computing by liquid-state NMR; (3) invented procedures, based on gradients combined with molecular diffusion, by which a wide variety of decoherent processes can be implemented using NMR; (4) used these procedures to perform the first demonstrations of quantum error correction as well as decoherence-free subspaces / systems; (5) used the average Hamiltonian techniques developed many years ago by John Waugh at MIT to implement the first simulations of one quantum system by another, as originally proposed by Richard Feynman. Many of the techniques we have developed in the course of this work promise to be highly useful in other approaches to quantum computing, both by our group as well as many others.

14. SUBJECT TERMS

15. NUMBER OF PAGES

16. PRICE CODE

| 17. SECURITY CLASSIFICATION OF REPORT | 18. SECURITY CLASSIFICATION OF THIS PAGE | 19. SECURITY CLASSIFICATION OF ABSTRACT | 20. LIMITATION OF ABSTRACT |
|---|---|---|---|
| UNCLASSIFIED | UNCLASSIFIED | UNCLASSIFIED | UL |

# 1. Foreword

This project was an essential component of a broader plan aimed at building the world's first scalable quantum computer. This plan calls for bootstrapping our way upwards through successively larger and more powerful QIP (quantum information processing) devices, each of which is used to discover the engineering principles needed to attain the next level. This process necessarily begins with natural systems (molecules in our case), and is expected to culminate in a computer architecture consisting of QIP modules which can be combined in a scalable fashion. Such a device has been mathematically proven to be capable of solving specialized but important computational problems that will forever be beyond reach of today's computer designs, including cracking RSA encryption and simulating experimentally inaccessible molecular, solid-state and nanoscopic systems **[26,27]**.

This report describes our successful completion of the first step of this journey, namely the construction of operational QIP devices, based on liquid-state NMR, together with the engineering principles that we have learned in the process. At the time we began this work, many excellent researchers doubted that quantum information processing would ever be possible **[28]**, and even today, liquid-state NMR remains the only technology capable of any substantial level of QIP on more than four qubits (quantum bits).

The question remains as to whether or not the laws of physics are compatible with scalable QIP devices, which can solve problems beyond what is possible with classical computers. This is a question which we will be able to explore in the course of the new research projects to which the liquid-state NMR project has led. The first of these, funded by the ARO (DAAD19-01-1-0519), is directed at attaining for the first a level of quantum control which brings us to the fault-tolerant threshold, at which arbitrarily long quantum computations become possible **[29,30]**. The second, funded by DARPA/DSO (MDA972-01-1-0003), is directed at building larger QIP devices, based on solid-state NMR, which can be prepared in a precisely known quantum state, thereby eliminating all ambiguity in the microscopic interpretation of the results **[31,32]**.

We now turn our attention to QIP devices based on liquid-state NMR, and how we have used them to demonstrate the essential ingredients of a quantum computer.

# 2. Contents, Figures and Tables

**Contents**



**Figures**

# 3. Project Report

## 3.A. Statement of the Problem

This project began in August of 1997. At that point in time, we had just published our first theoretical **[33]** and experimental **[34]** results indicating that Nuclear Magnetic Resonance (or NMR) spectroscopy on liquid organic compounds provides an astonishingly easy means of implementing simple quantum computations. To explain this, it is helpful to recall DiVincenzo's five criteria for any quantum information processor **[35]**, which state it must:

**(1)** Consist of well-defined and distinguishable two-state quantum systems (qubits).

**(2)** Admit a universal set of quantum gates from which all unitary operations can be built.

**(3)** Have an intrinsic decoherence rate that is slow compared to the gate operation time.

**(4)** Admit measurements of the states of the individual qubits w.r.t. a quantum basis.

**(5)** Be able to be prepared in a single known (or "fiducial") quantum state.

Liquid-state NMR has proven capable of meeting these criteria on a scale of a few qubits, as will now be described.

Many of the atomic nuclei in molecules have a "spin" of 1/2, and behave like tiny magnets. In a strong magnetic field, such nuclei constitute essentially perfect qubits, where the two states correspond to their alignment with or against the field. The magnetism from the "spins" in single molecules is far too weak to measure, but on placing a macroscopic sample of identical copies of the molecule in a magnetic field, the sum of the magnetism from the ensemble of all ca. $10^{20}$ spins together is fairly easy to detect. This is most conveniently done by measuring the radio-frequency (RF) signal that they generate as they precess about the applied magnetic field, in much the same way that a gyroscope precesses about a gravitational field. The strength of their magnetism, and hence the frequency with which they precess, depends upon their position in the molecule, making it possible to resolve each chemically distinct species of spin in the sample by its frequency.

Thus DiVincenzo's first criterion is fulfilled in liquid-state NMR quantum information processors by regarding all spins of a given chemical species in all the copies of the molecule in the sample as a single qubit. This is made possible by the fact that the spins in different molecules interact only very weakly, so that each molecule becomes an independent quantum computer and their duplication in the sample serves mainly to amplify the signal.

It turns out that the same RF "pulse sequences" that NMR spectroscopists have been using for decades to determine the structures of molecules can readily be adapted to implementing a universal set of quantum logic gates. Such RF pulses directly implement arbitrary single

qubit gates. By combining them with the natural "scalar coupling" interactions between chemically bonded pairs of spins, one can further implement the controlled-NOT gate, thereby obtaining a well-known universal set. Thus these systems also fulfill DiVincenzo's second criterion.

The third criterion is largely fulfilled almost gratis, since the nuclear spins in molecules in the liquid-state are extremely well-shielded from their surroundings, leading to decoherence times of hundreds of milliseconds - at least several times the time required to implement any single logic gate. While this is sufficient for many purposes, the decoherence rates of the spins in any given kind of molecule are determined by the underlying physics and not nearly long enough to reach the fault-tolerance threshold.

The fourth criterion is not only fulfilled by liquid-state NMR, but actually fulfilled in a way that is more convenient than it could be in a quantum computer that used single two-state quantum systems as its qubits. This is because the ensemble nature of the qubits used in liquid-state NMR not only increases the total signal, it also permits direct estimation of the expectation values of the microscopic observables over the random outcomes of a great many quantum measurements simultaneously. Such averages contain considerably more information than is contained in any one outcome, and hence such measurements allow one to determine the quantum state of the system with far fewer repetitions of the experiment than would otherwise be necessary. Moreover, this averaging process is very effective at filtering out <u>random</u> errors in the calculations during the final measurements; the strength of the signal is diminished by such errors, but there is usually signal to spare. The utility of ensembles justifies our introduction of the term "ensemble quantum computing" to emphasize it.

The fifth criterion was the most challenging to fulfill. This is because at the relatively high (compared to absolute zero) temperatures needed for liquid-state NMR, the spins in the molecules of the ensemble are in very nearly random states: in room temperature samples in the strongest superconducting magnets available, there is typically only about one-in-a-million more spins aligned with the magnetic field than against it. It was this problem, perhaps more than any other, which prevented the potential of NMR from being discovered earlier than it was. The problem, however, can again be solved by taking advantage of the ensemble nature of liquid-state NMR, together with the high level of control over the spins which is provided by pulse sequence technology.

Specifically, if one randomizes the spins in all molecules that are <u>not</u> in the desired state, then the aforementioned averaging effects will filter out the signal from those molecules, so that only those molecules whose spins are in the desired state can be seen. It is, of course, not possible to randomize the states of the spins via RF pulse sequences,

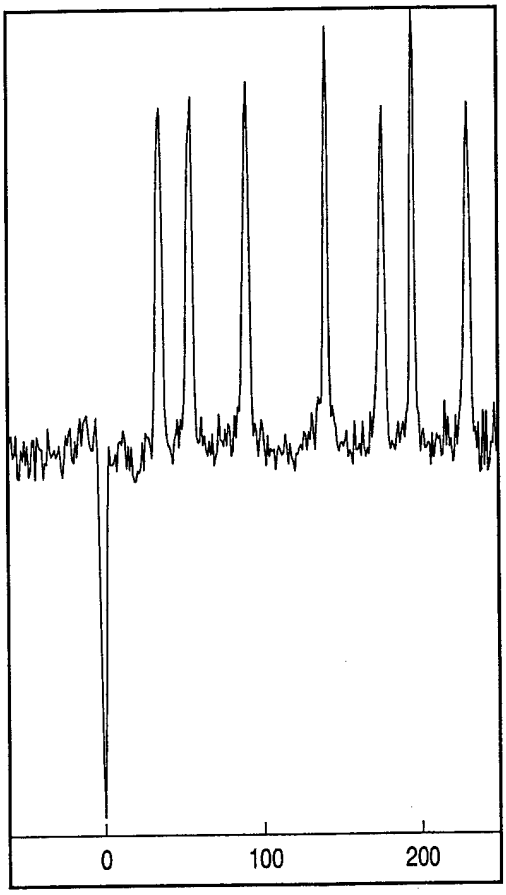
but NMR spectrometers are also equipped for gradient pulses, which vary the magnetic field across the sample and so randomly perturb the spins' states. By combining such gradient pulses with RF pulse sequences, it is possible to randomize the state of the spins selectively, based on their initial states, so that only those molecules wherein the spins are in the desired state are untouched. Unfortunately, the number of molecules whose spins are in the correct state declines rapidly with the number of kinds of spins, so that the signal available from such pseudopure ensembles becomes undetectable above about ten spins or so.

Our goals for this project have been to further refine the technology needed for ensemble quantum computing by liquid-state NMR spectroscopy, to use these methods to demonstrate all the essential ingredients needed to build a quantum computer by any technology, and thereby to determine a feasible trajectory towards larger, more convenient, and ultimately scalable quantum information processing devices. We now present our most important achievements towards fulfilling these goals.

## 3.B. Summary of the Key Results

**Design, analysis and optimization of quantum logic gates**

Although any universal set of quantum logic gates is sufficient for general quantum computing in principle, in any given physical situation some are bound to be far more efficient and/or practical than others. We have therefore developed theoretical methods, based on "geometric algebra", by which pulse sequences for any desired quantum logic gate can be designed **[1,4,12,14]**. These methods were first used to study implementations of the controlled-NOT gate by continuous frequency-selective RF irradiation in a two-spin system **[2]**, leading to the conclusion that this approach would probably not be competitive with discrete pulse sequences in most cases. Subsequently geometric algebra was used to obtain pulse sequences for all 16 inequivalent permutations of the states of a two-spin system **[6]**, and to study the potential of using the fact that multiple couplings among the spins are always active to implement multiple gates in parallel **[11]**.




Perhaps most spectacularly, pulse sequences were found by which a controlled$^n$-NOT gate could be implemented directly in time of order $n$, where

the superscript $n$ means that one spin was flipped conditional on the state of $n$ others **[7]**. An implementation of such "higher-order" gates using ordinary controlled-NOT gates would require many more operations as well as additional qubits for workspace. The experimental NMR spectrum obtained by applying a controlled$^3$-NOT gate to the equilibrium state of a four spin system is shown above. Each of the eight lines corresponds to one of the $2^3$ possible combinations of the other three spins up (parallel the field) or down (antiparallel). Thus it may be seen that the fourth spin has been flipped only in those molecules in which the other three are all antiparallel, as desired.

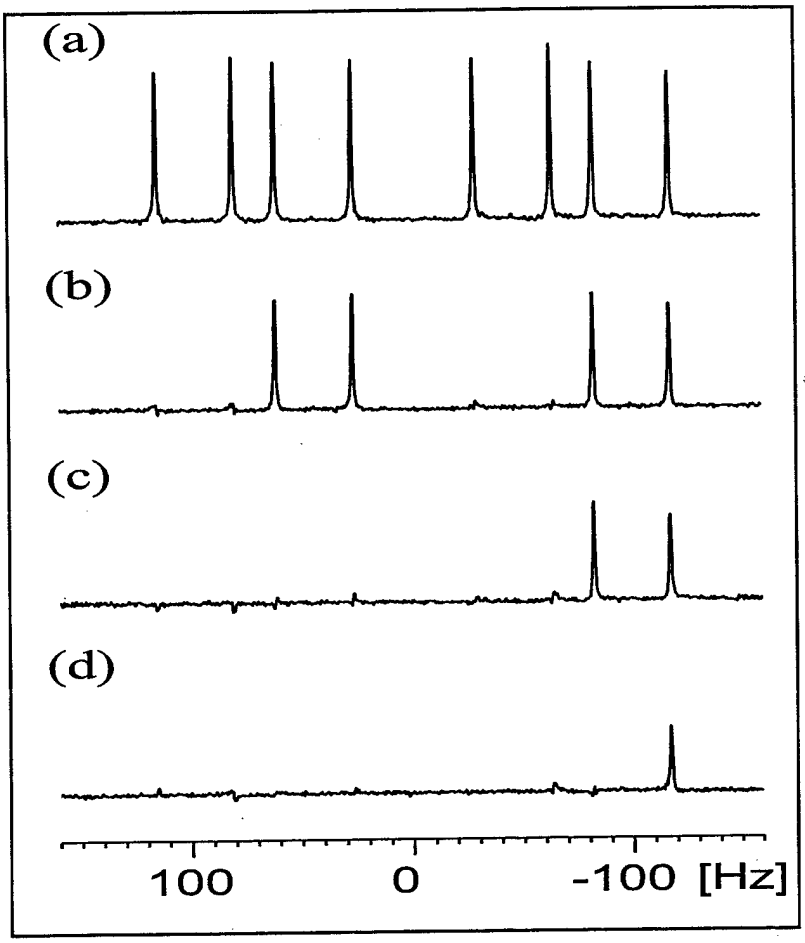
**Development and evaluation of methods for preparing pseudopure states**

As previously emphasized, the use of pseudopure ensembles is the key to emulating a quantum computer on an by liquid-state NMR starting from an equilibrium ensemble at room temperatures. There are essentially four different kinds of pseudopure ensembles, each of which is prepared from the equilibrium ensemble by a very different approach **[12]**, namely: **(i)** conditional pseudopure; **(ii)** relative pseudopure; **(iii)** temporal average pseudopure; and **(iv)** spatial average pseudopure ensembles.

The first of these, first used in **[36,37]** and subsequently rediscovered **[38]**, divides the spins up into "ancilla" and "functional" spins, and rearranges their states' populations so that all those molecules wherein the ancilla are in a given state also have their functional spins in a single state (on average over the sample). This method is efficient in terms of the number of ancilla, but has comparatively low signal-to-noise and becomes challenging to implement with large numbers of spins **[39]**. The second method also uses ancilla spins, but averages the states of the functional spins over the states of ancillae (mathematically, this corresponds to taking the "partial trace" over the ancillae). Although elegant in principle, a general procedure for any number of spins has not yet been found **[12]**.

The third type of pseudopure ensemble is a bit of a misnomer, because no single ensemble is prepared; rather, temporal averaging simply adds the spectra obtained from experiments starting with different permutations among all the spins' states save the desired one, so that the total signal from all other states averages towards zero **[40]**. This is similar to the use of phase cycling in NMR spectroscopy, but it is more labor intensive and hence has been used only with small numbers of spins. The last, developed by us **[34]**, uses magnetic field gradients to create a spatial variation in the state across the sample, such that the average over the sample is a pseudopure ensemble. Although convenient, it proved difficult to find a general method of preparing such pseudopure ensembles on any number of spins, and hence to analyze its efficiency in practice.

This was ultimately achieved by developing a preparation method that results in an ensemble which is essentially a combination of types **(i)** and **(iv)** above, or what we call spatial average conditionally pseudopure ensemble **[17]**. The efficiency with which it can be prepared from the equilibrium ensemble is illustrated by the sequence of spectra shown in the figure, whereby it may be seen that the signals from all possible states of the other spins save one are eliminated at an exponential rate. It is also possible to keep track of all the magnetization that is rendered unobservable in this process, and to recover that due to any desired pseudopure (sub)ensemble by suitable refocusing techniques.



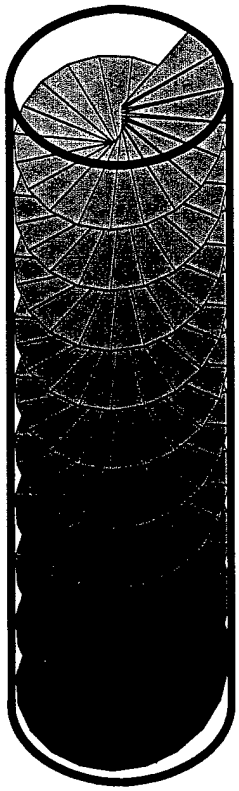

**Controlled decoherence via NMR gradient diffusion methods**

Decoherence is the greatest single obstacle to realizing quantum information processing by any technology. The comparatively long decoherence times with which Nature has blessed liquid-state NMR makes it ideally suited for studying methods of controlling decoherence, since additional decoherence can be induced in many ways. The important thing is to add it in a precisely known and controlled fashion, which can be systematically varied.

This was accomplished by taking well-established NMR methods for determining the rates at which the molecules in liquids diffuse, which work by measuring the rate of the decoherence due to the diffusion in a magnetic field gradient, and turning them around so as to obtain a known decoherence rate from a known diffusion rate. Specifically, the application of a magnetic field gradient causes the spins to precess at differing rates, depending upon their position in the NMR sample tube. This winds the spin's directions into a spiral, as shown on the right below. The average magnetization across the sample is rapidly goes to zero, because equal numbers of spins are pointing in all directions. The gradient field is then turned off for a fixed period of time, during which molecular diffusion "blurs" the spiral. The direction of the gradient is then reversed, which unwinds

the residual spiral and "refocuses" the magnetization it contains. The rest of irreversibly lost, or "decohered". By varying the period of time in which the diffusion occurs, one can obtain any desired amount of decoherence.

This implements what is known as collective decoherence, because the spins in every molecule are randomized together in the same way (by diffusion). It is possible, however, to wind up only one (kind of) spin at a time into a spiral, allow time for diffusion, and then refocus, thereby decohering each spin independently. It is even possible to decoher the spins at differing rates, or with any desired correlations among them. This versatility proved extremely useful in our demonstrations of quantum error correction (see below).



In order to quantitatively analyze these processes, and to relate them to the usual (Lindblad & Kraus) formulae used to describe decoherence in quantum theory, we found it convenient to extend our geometric algebra formalism for the design NMR pulse sequences, so that the extended formalism could also describe gradient-diffusion induced decoherence **[22]**. This extension is based upon the well-known Hadamard matrix product. Its convenience stems from its commutativity, its the mixed product formula with tensor product, and that it allows the space-time dependence to be factored out of the expressions. It also, needless to say, has a simple interpretation within geometric algebra.

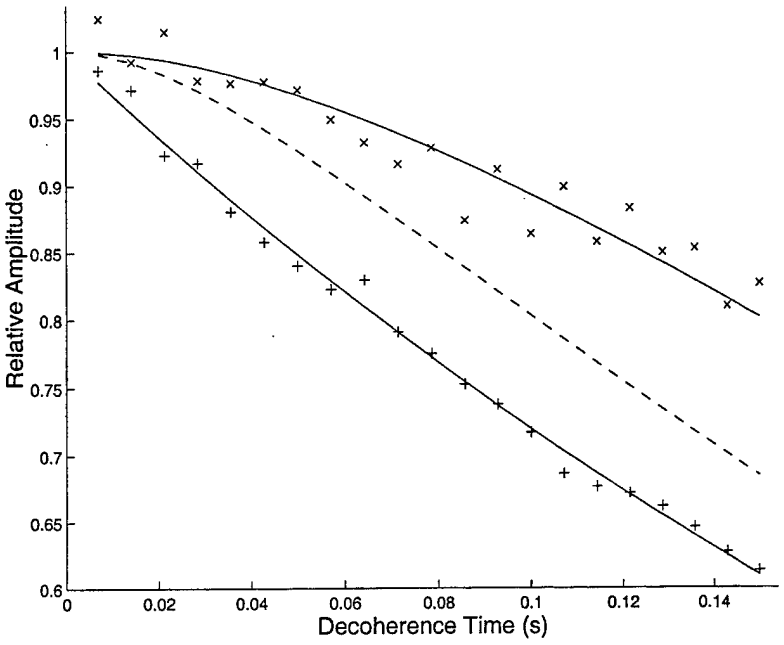
**Demonstration of a quantum error correcting code**

Because they are intrinsically analog devices whose states "drift" in the presence of even very small random errors, it is certain that any large-scale quantum information processing device will need some form of active error correction. This incurs a very high overhead (at least quintupling the number of qubits needed), and hence passive error-avoiding encodings are also expected to play an important role in reaching the "fault-tolerant" threshold at which arbitrarily long, error-free calculations become possible with active error correction.

These facts, together with our unique ability to introduce controlled decoherence, led us to focus on demonstrating a quantum error correcting code at an early stage of this project. In this we were greatly assisted by two experts in the field, Raymond Laflamme and Emanuel Knill at Los Alamos. This collaboration resulted in the first demonstration of a quantum error correcting code, which at the time was also the most complex quantum algorithm to be implemented on an NMR quantum information processor **[3]**. This demonstration utilized the spins in commercially available $^{13}C$-labeled alanine, together with the natural

decoherence processes operative in this molecule. Additionally, each of the product operator components of the encoded state was subjected to gradient-diffusion decoherence, allowing a very precise demonstration of the inhibition of collective decoherence by error correction.

Subsequently, a much more detailed study of the same three-qubit error correcting code was made, again on alanine, but this time fully carrying out the encoding, decohering, decoding and correction steps, and at the same time testing the code with both collective and independent gradient - diffusion decoherence **[13]**. Additionally, a closed-form expression was derived by geometric algebra methods for the error-corrected decay of the magnetization as a function of the correlations in the decoherence processes operative at the three spins. These theoretical curves for independent and collective (dashed) decoherence are shown in the figure, together with the independent and uncorrected data points. This demonstrates that quantum error correcting codes can not only inhibit decoherence, but that they can also be used to probe the mechanism of decoherence operative in any given case.

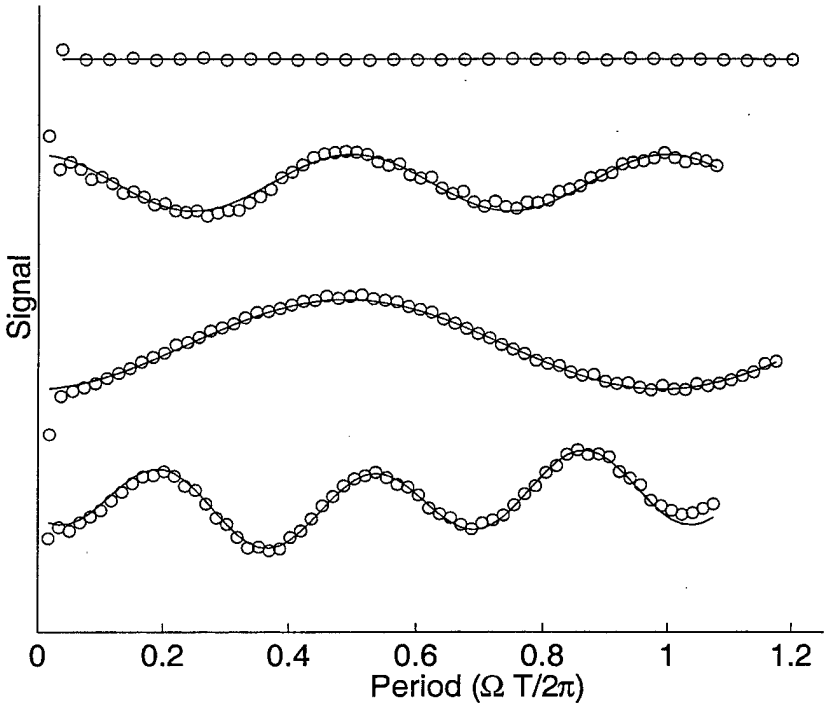



**Quantum simulation, with and without decoherence**

It was first observed by R. P. Feynman that while the exact simulation of quantum systems on a classical computer requires exponential time (and memory, for all practical purposes), it should be possible to make one quantum system simulate another far more efficiently. It was later shown by S. Lloyd that a quantum computer, as conceived by Deutsch and Jozsa, was well-suited to serve as a universal quantum simulator which could efficiently simulate any other quantum system. Up until this project, however, no one had actually done it, or even worked out a specific protocol for any given case.

In this case we found another standard NMR technique, called average Hamiltonian theory (AHT) and first developed by J. Waugh at MIT, was ideally suited to the problem. Our first example, of course, was a quantum harmonic oscillator, truncated after the first four levels since that was all that could be simulated with the two-spin system (dibromo-thiophene) that we used. The pulse sequence obtained from AHT included time delays which

could be varied to change the amount of time simulated, after which a spectrum was collected to monitor the evolution of the oscillator. The results are shown in the figure on the right below for various initial states, which resulted in frequencies of oscillation varying by integer multiples exactly as predicted. Similar simulations were also performed for a damped and driven quantum harmonic oscillator **[5]**.




To further emphasize the versatility of these simulations, we subsequently simulated a three-particle interaction, which does not occur in nature (since all elementary forces are between two particles) **[10]**. We further went on to include decoherence in such simulations. Although this could certain be done using gradient-diffusion methods, multi-body forms of decoherence such as the nuclear Overhauser effect cannot be obtained via this approach. For this reason we developed methods, akin to average Liouvillian theory, by which the natural relaxation superoperator could be modified during simulations as above, so as to mimic more complex forms of decoherence in the simulated system. The simulation of systems beyond reach of today's computers will however require upwards of twenty qubits, and must wait until the next generation devices come on line **[18]**.

**Further Achievements**

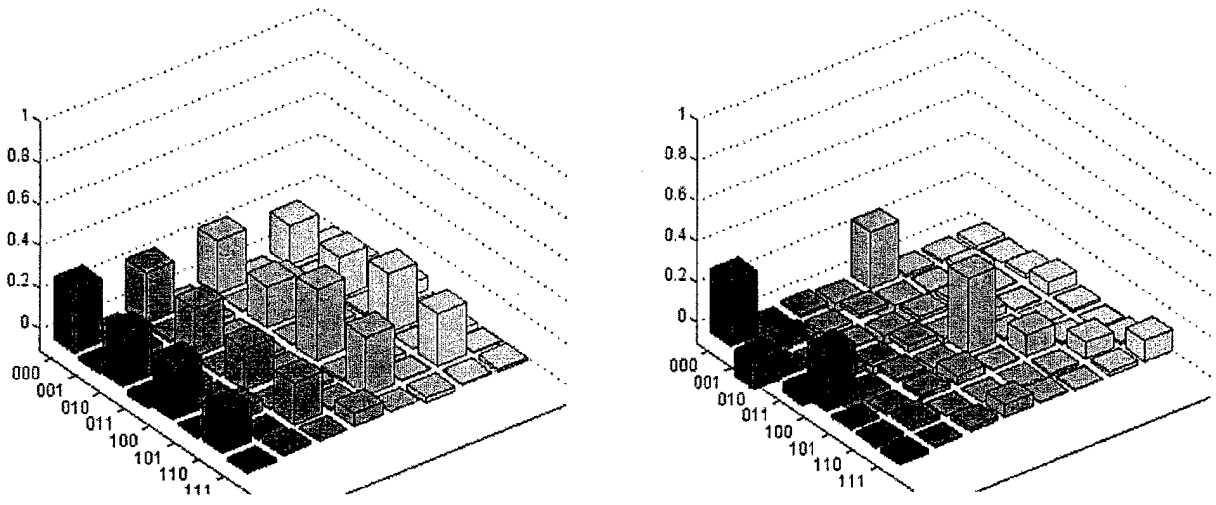
In addition to the above major milestones, a number of less quantifiable but nevertheless important results have been obtained. Foremost among these are the improvements in the underlying hardware, software and methodology available, which have permitted steady increases in the efficiency and precision with which these experiments can be performed. Although implemented by us only for NMR, many of these improvements can potentially be transferred to other proposed implementations of QIP.

Additionally, we have been able to develop quantum codes which specifically correct for two-body interactions among qubits, rather than with external random fields **[16]**. Although one can achieve the same effect via concatenation **[29,30]**, it is more efficient to code directly for such interactions whenever they are known to occur, as is likely to be the

case in many quantum computer implementations. We have also demonstrated the existence of the phenomenon of stochastic resonance by NMR, which provides a means studying the system's intrinsic relaxation dynamics **[19]**, as well as the principles of coherent quantum feedback **[9]**, and of information transmission through a quantum channel **[20]**.

On the simulation side, we have prepared the pseudopure analog of an entangled GHZ state **[8]**, and demonstrated an advanced "quantum eraser" effect in which not only interference, but also entanglement, is restored by suitable strong measurements. Although strong measurements are not available in ensembles, magnetic field gradients were able to erase the same information and hence reveal coherences which, in an isolated quantum system, would be taken as indicative of entanglement **[24]**. Finally, we have implemented a three-qubit quantum Fourier transform (QFT) by NMR **[21]**, which is an essential component of several quantum algorithms. We are now using it both as a benchmark for coherent control, and as a means of studying the quantum dynamics of classically chaotic systems.

The results of tomography before and after the QFT are shown in the figure below, where the left-hand plot shows the coherences (density matrix elements) of a pseudopure ensemble in a superposition over its even states, while the right-hand illustrates that the QFT revealed this underlying periodicity by putting coherence into state number $4 = 2^3/2$.



## 3.C. List of Publications and Technical Reports

**1.** S. S. Somaroo, D. G. Cory and T. F. Havel, "Expressing the operations of quantum computing in multiparticle geometric algebra", Phys. Lett. A. **240:1-7**, 1998.

**2.** D. G. Cory, A. E. Dunlop, T. F. Havel, S. S. Somaroo and W. Zhang, "The Effective Hamiltonian of the Pound-Overhauser Controlled-NOT Gate", Los Alamos National Labs preprint archive **quant-ph / 9809045**, 1998.

**3.** D. G. Cory, W. Maas, M. Price, E. Knill, R. Laflamme, W. H. Zurek, T. F. Havel and S. S. Somaroo, "Experimental Quantum Error Correction", Phys. Rev. Lett. **81:2152-2155**, 1998.

**4.** T. F. Havel, S. S. Somaroo, C.-H. Tseng and D. G. Cory, "Ensemble quantum computing by NMR spectroscopy: Product operators, pseudo-pure states, and an implementation of quantum error correction", Proc. SPIE **3385:72-83**, 1998.

**5.** S. S. Somaroo, C.-H. Tseng, T. F. Havel, R. Laflamme and D. G. Cory, "Quantum simulations on a quantum computer", Phys. Rev. Lett. **82:5381-5384**, 1999.

**6.** M. D. Price, S. S. Somaroo, C.-H. Tseng, J. C. Gore, A. F. Fahmy, T. F. Havel and D. G. Cory, "Construction and implementation of NMR quantum logic gates for two-spin systems", J. Magn. Reson. **140:371-378**, 1999.

**7.** M. D. Price, S. S. Somaroo, A. E. Dunlop, T. F. Havel and D. G. Cory, "Generalized (controlled)$^n$-NOT quantum logic gates", Phys. Rev. A **60:2777-2780**, 1999.

**8.** R. J. Nelson, Y. Weinstein, D. G. Cory and S. Lloyd, "Experimental demonstration of Greenberger-Horne-Zeilinger correlations using nuclear magnetic resonance", Phys. Rev. A **61:002106** (2000).

**9.** R. J. Nelson, D. G. Cory and S. Lloyd, "Experimental demonstration of fully coherent quantum feedback", Phys. Rev. Lett. **85:3045-8** (2000).

**10.** C.-H. Tseng, S. S. Somaroo, Y. Sharf, E. Knill, R. Laflamme, T. F. Havel and D. G. Cory, "Quantum simulation of a three-body interaction Hamiltonian on an NMR quantum computer", Phys. Rev. A **61:012302**, 2000.

**11.** M. D. Price, T. F. Havel and D. G. Cory, "Multi-qubit logic gates in NMR quantum computing", New J. Phys. **2:10**, 2000.

**12.** T. F. Havel, S. S. Somaroo, C.-H. Tseng and D. G. Cory, "Principles and demonstrations of quantum information processing by NMR spectroscopy", Applic. Algebra in Engin. Commun. & Comput. **10:339-374**, 2000.

**13.** Y. Sharf, D. G. Cory, S. S. Somaroo, T. F. Havel, E. Knill, R. Laflamme and W. H. Zurek, "A study of quantum error correction by geometric algebra and liquid-state NMR spectroscopy", Molecular Physics **98:1347-63**, 2000.

**14.** T. F. Havel, D. G. Cory, S. S. Somaroo and C.-H. Tseng, "Geometric algebra methods in quantum information processing by NMR spectroscopy", in Advances in Geometric Algebras with Applications (E. Bayro-Corrochanno & G. Sobczyk, eds.), Birkhauser, Boston, MA, 2000.

**15.** C.-H. Tseng, S. S. Somaroo, Y Sharf, E. Knill, R. Laflamme, T. F. Havel and D. G. Cory, "Quantum simulation with natural decoherence", Phys. Rev. A **62:032309**, 2000.

**16.** Y. Sharf, T. F. Havel and D. G. Cory, "Quantum codes for controlling coherent evolution", J. Chem. Phys. **113:10878-85**, 2000.

**17.** Y. Sharf, T. F. Havel and D. G. Cory, "Spatially encoded pseudo-pure states for quantum information processing", Phys. Rev. A **62:052314**, 2000.

**18.** D. G. Cory, R. Laflamme, T. F. Havel, E. Knill, S. Lloyd, M. Pravia, Y. Sharf, G. Boutis, E. Fortunato, Y. Weinstein and G. Teklemariam, "NMR-based quantum information processing", Prog. Phys. (Fortschritte der Physik) **48:875-907**, 2000.

**19.** L. Viola, E. M. Fortunato, S. Lloyd, C.-H. Tseng and D. G. Cory, "Stochastic resonance and nonlinear response using NMR spectroscopy", Phys. Rev. Lett. **84:5466-9**, 2000.

**20.** M. D. Price, E. M. Fortunato, M. A. Pravia, C. Breen, S. Kumaresean, G. Rosenberg and D. G. Cory, "Information transfer on an NMR quantum information processor", Concepts in Magn. Reson. **13:151-8** (2001).

**21.** Y. S. Weinstein, M. A. Pravia, E. M. Fortunato, S. Lloyd and D. G. Cory, "Implementation of the Quantum Fourier Transform", Phys. Rev. Lett., **86:1889-91**, 2001.

**22.** T. F. Havel, Y. Sharf, L. Viola and D. G. Cory, "Hadamard products of product operators and the design of gradient-diffusion experiments for simulating decoherence by NMR spectroscopy", Phys. Lett. A **280:282-288**, 2001.

**23.** T. F. Havel and C. Doran, "Geometric algebra in quantum information processing", Quantum Computation and Quantum Information Science (Contemporary Math. Series, Am. Math. Soc., Providence, RI), in press, 2001.

**24.** G. Teklemariam, Y. Sharf, C.-H. Tseng, T. F. Havel and D. G. Cory, "An NMR analog of the quantum entanglement eraser", Phys. Rev. Lett. **86**, in press, 2001.

**25.** T. F. Havel, "Qubit logic, algebra and geometry", in *Automated Deduction in Geometry* (D. Wang and J. Richter-Gebert, eds.), Lect. Notes Artif. Intel. **2061**, in press, 2001.

## 3.D. Scientific Personnel

**(1)** Timothy F. Havel (P.I.), Ph.D. U. C. Berkeley, 1982.

**(2)** David G. Cory (P.I.), Ph.D. Case Western Reserve, 1987.

**(3)** Shyamal Somaroo (Postdoc.), Ph.D. Univ. of Cambridge, England, 1996.

**(4)** Ching-Hua Tseng (Postdoc.), Ph.D. Harvard Univ., 1997.

**(5)** Yehuda Sharf (Postdoc), Ph.D. Technion, Isreal, 1998.

**(6)** Mark Price (Graduate Student), Ph.D. MIT, 1999.

**(7)** Evan Fortunato (Graduate Student), Ph.D. MIT, expected 2002.

**(8)** Marco Pravia (Graduate Student), Ph.D. MIT, expected 2002.

**(9)** Grum Teklemariam (Graduate Student), Ph.D. MIT, expected 2002.

**(10)** Yaakov Weinstein (Graduate Student), Ph.D MIT, expected 2003.

**(11)** Amy Dunlop (Graduate Student), M.S. MIT, 1998.

## 4. Report of Inventions

None.

## 5. Bibliography (continued from 4.C)

**26.** C. H. Bennett and D. P. DiVincenzo, "Quantum Information and Computation", Nature **404:247-55** (2000).

**27.** M. Brooks, ed., Quantum Computing and Communications, Springer-Verlag (1999).

**28.** R. Landauer, "The physical nature of information", Phys. Lett. A **217:188-93** (1996).

**29.** A. M. Steane, "Introduction to quantum error correction", Phil. Trans. R. Soc. Lond. A **456:1739-58** (1998).

**30.** D. Gottesman, "Introduction to quantum error correction", AMS Annual Meeting, Short Course on Quantum Computation (January, 2000); see LANL preprint **quant-ph/0004072**.

**31.** S. L. Braunstein, C. M. Caves, R. Jozsa, N. Linden, S. Popescu and R. Schack, "Separability of very noisy mixed states and implications for NMR quantum computing", Phys. Rev. Lett. **83:1054-7** (1999).

**32.** R. Schack and C. M. Caves, "A classical model for bulk-ensemble quantum computation", Phys. Rev. A **60:4354-62** (1999).

**33.** D. G. Cory, A. F. Fahmy and T. F. Havel, "Ensemble quantum computing by nuclear magnetic resonance spectroscopy", Proc. Natl. Acad. Sci. USA **94:1634-9** (1997).

**34.** D. G. Cory, M. D. Price and T. F. Havel, "Nuclear magnetic resonance spectroscopy: An experimentally accessible paradigm for quantum computing", Proc. 4th Workshop on Physics and Computation (T. Toffoli, M. Biafore and J. Leao, eds.), pp. 87-91 (New England Complex Systems Institute, Boston MA, 1996); formally published in a Special Quantum Computing Issue of Physica D **120:82-101** (1998).

**35.** D. P. DiVincenzo, "The physical implementation of quantum computation", Fort. Phys. **48:771-83** (2000).

**36.** M. E. Stoff, A. J. Vega and R. W. Vaughan, "Explicit demonstration of spinor character for a spin 1/2 nuclear via NMR interferometry", Phys. Rev. A **16:1521-4** (1977).

**37.** D. Suter, A. Pines and M. Mehring, "Indirect phase detection of NMR spinor transitions", Phys. Rev. Lett. **57:242-4** (1986).

**38.** N. Gershenfeld and I. L. Chuang, "Bulk spin-resonance quantum computation", Science **275:350-6** (1997).

**39.** L. M. K. Vandersypen, C. S. Yannoni, M. H. Sherwood and I. L. Chuang, "Realization of logically labeled effective pure states for bulk quantum computation", Phys. Rev. Lett. **83:3085-8** (1999).

**40.** E. Knill, I. Chuang and R. Laflamme, "Effective pure states for bulk quantum computation", Phys. Rev. A **57:3348-63** (1998).